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Absence of localization in disordered and hierarchical lattices : an overview

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Abstract : Usually the notion of an extended wavefunction is associated with a periodic lattice Bloch function is a classic example On the other hand, if randomness is introduced in a lattice, wave functions are, in general, exponentially localized, as was pointed out by Anderson in 1958. Perhaps the most striking change in the character of electron-states occurs in one dimension where, according to Anderson, almost all the single particle states are exponentially localized for any amount of disorder However around 1989, it was pointed out that short-ranged positional correlation between the constituent atoms in the model of a binary alloy may give rise to extended electronic states (and therefore large conductivity) in an otherwise random system This was shown using a one dimensional model of an alloy where, the effect of disorder is known to be strongest In this talk we will reivew the basic things about this latter phenomenon, which is sometimes called resonance. We will first illustrate the case of a linear chain with 'correlated' disorder, and then extend the idea to a group of quasiperiodic chains (only one member of the group will however, be discussed) and some hierarchical lattices

Keywords Localization, quasiperiodicity, fractals

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1. Introduction

Localization of one electron eigenstates in a system with random disorder is an old problem. Anderson [1] observed that electron localization is caused by coherent superposition of waves scattered from randomly placed sites in a lattice. Of course, one can not ignore the other major factors, like the phonons or the many-electron effects, but the simple non-interacting picture of electron localization, as proposed by Anderson way back in 1958, still continues to generate interest. Within a tight binding formalism a clear physical picture emerges for various properties of different models of disorder (and for 'deterministic' disorder, as will be discussed later).

One striking result is that in a one dimensional system, almost all the one-electron eigenstates are exponentially localized for any amount of disorder. The amplitude of the single particle wavefunction $\psi(x)$ drops off as $\exp(-\lambda x)$ as one moves along the chain from any given site. λ is the inverse of the localization length. This is in sharp contrast to the character of electronic states in a periodic lattice, where, it is well known, that the solutions are Bloch functions (of the form $\exp(ikx)\, U_k(x)$, $U_k(x)$ is a periodic function having the periodicity of the lattice), perfectly extended over the entire lattice. Thus, we may associate extended eigenfunctions with perfect long range translational order, and exponentially localized states with broken translational order, more specifically with the presence of random disorder. The remaining part of our discussion will mainly focus on the possibility of obtaining extended type of electronic states in systems where there is no translational periodicity [2, 3]. We shall talk only about what happens in one dimension (or nearly one dimension), not only because we can get exact results in several cases, but also because of the fact that recent advancement in nanostructure technology has enabled us to fabricate nearly one dimensional superlattices where one can test the theoretical predictions, and look for possible applications as well.

2. A simple model of correlated disorder

In this section we describe the essential results obtained by Dunlap *et al* [2] who examined the possibility of a *de-localization* of electronic states in a simple model. Suppose, we have a string composed of two types of 'atoms' A and B placed equal distance apart. We are interested in configurations in which B always

comes in pairs. However, a pair $B-B$ is distributed in a completely random fashion on the host A lattice. A typical configuration may be .....$A-B-B-A-A-A-B-B-B-B-A-B-B-A-A-A$.... and so on. This arrangement is a slight variation of a random binary alloy model. But it is interesting to note that this seemingly innocent restriction on the distribution of the B's may have a profound impact on the very character of the electronic state at a special value of the energy. Let us try to clarify this statement. We consider the standard tight binding hamiltonian :

$$H = \sum_i \varepsilon_i |i\rangle\langle i| + \sum_{<ij>} \left[t_{ij} |i\rangle\langle j| + t_{ji} |j\rangle\langle i| \right], \tag{1}$$

where ε_i is the on-site potential at the i-th atomic site, and $t_{ij} = t_{ji}$ is the nearest neighbour hopping integral. Solving the time independent Schrodinger equation in our case reduces to finding the solutions of a set of difference equations having the form

$$(E-\varepsilon_n)\psi_n = t_{n,n+1}\psi_{n+1} + t_{n,n-1}\psi_{n-1}, \tag{2}$$

where ψ_n is the amplitude of the wave function on the n-th site and $t_{n,n+1}$ is the nearest neighbour hopping integral. Let us address the problem of 'diagonal' disorder, *i.e.* we set $t_{ij} = t_{ji} = t, \varepsilon_i$ being the random variable which can assume two values, *viz.*, ε_A and ε_B. In our discussion the values ε_B always occur pairwise. Using the set of difference eq (2), one can write

$$\begin{pmatrix} \psi_{n+1} \\ \psi_n \end{pmatrix} = \prod_{i=1}^{n} M_i \begin{pmatrix} \psi_1 \\ \psi_0 \end{pmatrix}, \tag{3}$$

with $\psi_1 = 1$ and $\psi_0 = 0$. The matrices M_i are given by

$$M_i = \begin{pmatrix} (E-\varepsilon_i)/t & -1 \\ 1 & 0 \end{pmatrix}. \tag{4}$$

The product of the transfer matrices for the random dimer model (RDM) turns out to be .... $M_A \cdot M_B \cdot M_B \cdot M_A$ .. and so on. Now, we observe that the pair of matrices $M_B \cdot M_B$ becomes equal to an identity matrix (apart from a negative sign) for a very special value of the energy, *viz.*, $E = \varepsilon_B$. If we now select the site energies for this model such that $-2t < \varepsilon_B - \varepsilon_A < 2t$, then we have an extended eigenstate for the system. This happens as a result of a *resonance* [4]. At that particular energy (and hence, at a particular value of the wave vector), the scattering from the second member of the dimer is 180° out of phase from the scattering from the first member. As a result, the electron *feels* an array of A-sites only. This results in completely unattenuated transmission at $E = \varepsilon_B$. However, it should be appreciated that the wavefunction, though extended, is not a Bloch function. This model was initially proposed to explain some abrupt enhancement in the dc-conductivity in polyanilines on protonation [5].

Before we end, two points are to be noted : (i) It is absolutely essential that we have a 'dimer' or an 'n-mer' in general to have any kind of resonance. That is, the 'impurity' must have an internal structure [2]. Otherwise the product transfer matrix can not be made equal to an identity matrix and an unattenuated transmission of an incident wave packet will not be possible. (ii) In the general case of n impurities placed side by side, one can write $M_B^n = U_{n-1}(x_B)M_B - U_{n-2}(x_B)I$ where, U_n is the Chebyshev polynomial of the second kind, $x_B = trace(M_B)/2$ and I is the identity matrix. The resonance condition is easily satisfied by making $U_{n-1}(x_B) = 0$ from which one can extract the eigenvalues for which the system supports extended eigenstates.

3. Extended states in quasiperiodic lattices

Similar resonance phenomena are also observed in aperiodic but deterministic sequences where, by the very method of construction short range positional correlations appear at all scales of length. Let us consider a specific example, *viz.*, the Thue-Morse lattice. The lattice is constructed by inflating a basic *seed* A by replacing A by a pair AB and B by a pair BA in successive generations. A typical chain in the 5-th generation, say, looks like $ABBA\ \underbrace{BAABBAAB}\ ABBA$, where, we have emphasized the 'dimer' correlations with an underbrace. Similar dimers appear in all generations. Since the product matrix across one member of the dimer, *i.e.* $BAAB$, has the same trace as that for the product $ABBA$ (cyclic invariance of trace) which form the two flanks of the above generation, the entire matrix-product becomes equal to identity for those energy values at which the trace of matrix M_{BAAB} vanishes. Similar dimers of bigger and bigger lengths can be identified with increasing generations.

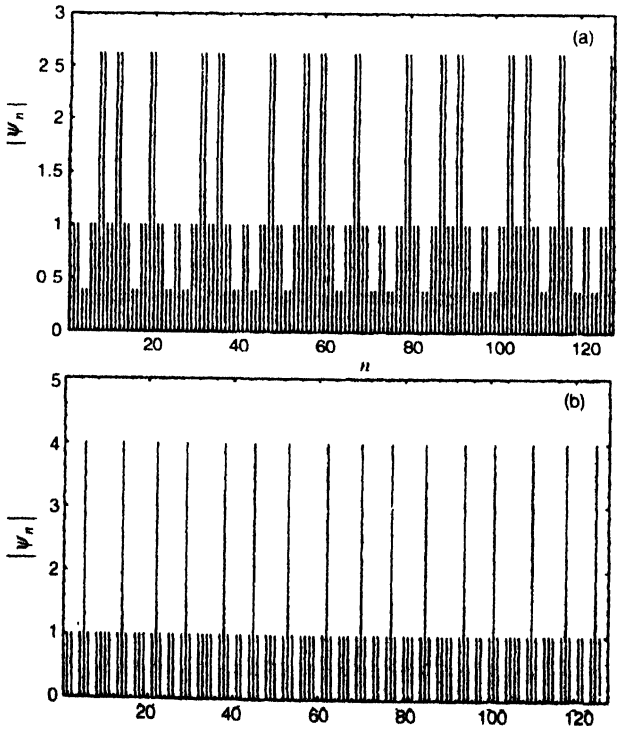

Figure 1. Distribution of amplitudes for typical extended states in a TM chain.

and the desired energy values can be obtained by setting the trace of the dimer matrix equal to zero at any length scale. This implies solving polynomial equations in energy E, the degree of the polynomial increasing with higher generation lattices. Thus, for an infinite Thue-Morse (TM) chain, one unravels a (countable) infinity of extended eigenstates. One can arrive at the same conclusion in another way, by determining the conditions for which the block matrices of the structure $M_{ABB\,AB\,AAB}$ and $M_{B\,AAB\,ABBA}$ commute with one another [6] in different generations. These states do not form 'bands' in the sense of ordered lattices, but, are generally very closely spaced, giving sometimes the flavour of a quasicontinuous distribution of eigenvalues. In this particular case, since the product transfer matrix at resonance becomes precisely equal to an identity matrix (at any generation), we obtain completely unattenuated transmission for arbitrarily large TM lattices (for the resonance states). We show in Figure 1 amplitudes of typical extended states in a TM lattice. Similar extended states (infinite in number) are observed in the infinite generalised Fibonacci chains [7], generated following the prescription $A \rightarrow AB^n$ and $B \rightarrow A$ with $n \geq 2$. The mode of analysis is same as above. The self-similarity again plays a crucial role in the existence of an infinite number of such states.

4. Hierarchical lattices

We will discuss two specific examples involving two models of regular fractals, which have been very popular over the years for studying critical properties. These are the non-branching Koch fractal [8] and the Vicsek fractal [9]. These structures offer many features similar to those occurring in actual disordered systems, and at the same time it is possible to do exact analytical calculations for many of them. Hence, the interest is quite obvious. We, in particular, will focus on two other aspects of our problem of interest. In the first example, we investigate the role played by an external magnetic field in the existence of extended type states in a fractal, and in the second example, we show that one encounters situations where extended states may arise even when there is no apparent 'dimer'-like correlations in a lattice. The character of these states however, is quite different from those occurring in the quasiperiodic chains, the difference showing up in the behaviour of the transmission coefficient for large finite lattices.

(i) A non-branching Koch fractal in a magnetic field :

The second generation fractal is shown in Figure 2(a). We introduce a magnetic field in a direction perpendicular to the plane of the paper. The flux enclosed by an elementary triangle is ϕ, say. The purpose of having a magnetic field will become clear as we proceed. As a result of this field, the time reversal symmetry is broken for an electron when it hops around the triangular plaquette. This is taken care of by fixing a phase factor with hopping integral, $te^{\,i\gamma/N}$ for *forward* hopping, and, $te^{\,-i\gamma/N}$ for 'backward' hopping in the tight binding Hamiltonian [10]. N being the number of sites in the plaquette. Here, $\gamma = 2\pi\phi/\phi_0$, ϕ_0 being equal to hc/e, the flux quantum. Figure 2(b) shows how this hierarchical structure can be reduced to an effectively one dimensional chain by decimating the D-type vertices. The renormalized site energies are $\tilde{\varepsilon}_C = \varepsilon_C + 2t_2^2/(E-\varepsilon_D)$ and, $\tilde{\varepsilon}_B = \varepsilon_B + 2t_2^2/(E-\varepsilon_D)$. The dimer-type correlation is obvious from the Figure. The sites $\tilde{B}$ or $\tilde{C}$ form dimers. If we now desire that $E = \tilde{\varepsilon}_B$, then the product transfer matrix for the effective pair of $\tilde{B}$ sites is identity, and we have an ordered sequence of $\tilde{C}\tilde{C}A$ (identified as an α-type block in Figure 2(b)). However, according to what we have discussed so far, the trace of the transfer matrix for such a unit $\tilde{C}\tilde{C}A$ has to be bounded by two in order that the above energy corresponds to an extended eigenstate. Now the trace is a function of the external flux. We plot the value of half the trace (which should be ≤ 1) against different values of the flux (Figure 3). We find that, the trace-condition is satisfied only at some specific values of the magnetic flux ! It can be shown that, for $E = \tilde{\varepsilon}_B$ and for these special values of the flux, Koch fractals of any arbitrary size become completely transparent to an incoming electron [11].

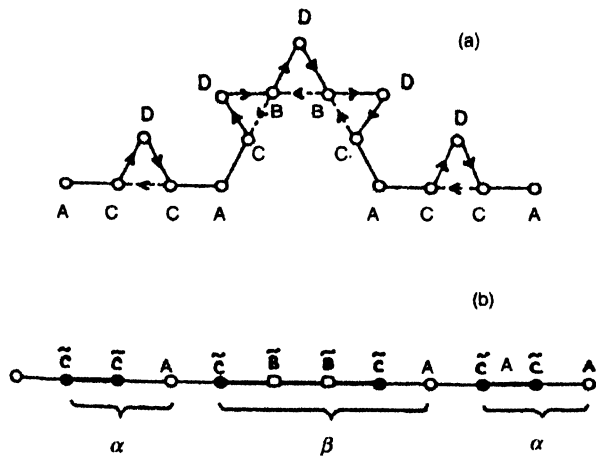

Figure 2. (a) Portion of a non-branching Koch fractal, and, (b) the effective one dimensional chain by decimating the 'D' vertices

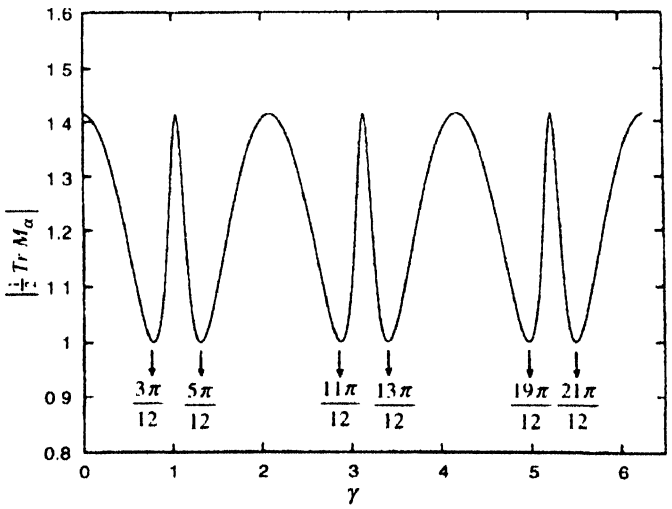

Figure 3. Variation of $(\mathrm{TrM}_\alpha)/2$ against magnetic flux

The analysis for extended states can be made in another way. In Figure 2(b) we identify two clusters labelled by α and β. It can be shown that, the transfer matrices for these two clusters, *viz*, M_α and M_β commute with each other provided $E(E^2-2)(E+2\cos 3\gamma)=0$. Thus, if we have an infinite fractal, then for any of the four energy values obtained from the above equation, it is possible to arrange the α and β blocks in any sort of periodic fashion, and thus one can expect extended eigenstates But what happens to the transmission coefficient across large finite versions of the fractal lattice at these energies? Let us discuss just one case, which is E=0. It can be shown [11] that the value of the transmission coefficient for an l-th generation Koch fractal is given by

$$T(l)=\frac{1}{1+(4N_l-3)^2\cos^2 3\gamma}, \tag{5}$$

N_l is the number of sites in the l-th generation. We thus find that though the states may be extended in the sense that the amplitudes of the wavefunction remains non-zero even at the farthest part of the lattice, the transmission coefficient may behave anomalously, sometimes decaying in a power-law fashion with the system-size.

(ii) A Vicsek fractal :

The seed for generating this fractal is a five site cluster. The next generation is obtained by joining identical clusters at each of the five extremeties of the seed (Figure 4). The fractal grows in this fashion. In this case, there is no 'dimer'-like positional correlation. However, it has been shown [12] that an infinitely large fractal can support an infinity of extended eigenstates. For some specific energy eigenvalues, it is possible to solve the Schrödinger equation consistently over any arbitrarily large lattice. One considers a five-site plaquette at the lowest length scale, and forces the value of the amplitude to be equal to zero at the central site of the plaquette. The idea is then extended to larger scales of length. Extended states are found to have energy eigenvalues given by the equation,

$$E=\varepsilon_b(n)\pm T, \tag{6}$$

where ε_b is the site energy of the extreme site at the n-th stage of renormalization, and T is the hopping integral between the extreme sites of two neighbouring clusters. The amplitudes of the wavefunctions for two different cases are shown in Figure 4. One can observe, that at the bare length scale, amplitude is zero at the centre of the smallest five-site cluster. However, in this case also, an analysis of the renormalization group equations prove [12] that such extended states exhibit a decaying transmission (with system size).

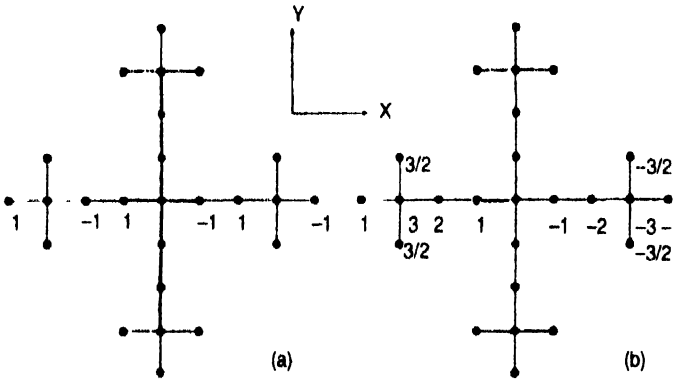

Figure 4. Variation of $(TrM_\alpha)/2$ against magnetic flux

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